Final Technical Report

DEVELOPMENT OF AN ADVANCED FLUID MECHANICS MEASUREMENT FACILITY FOR FLAME STUDIES OF NEAT FUELS, JET FUELS, AND THEIR SURROGATES

(AFOSR Grant FA9550-08-1-0289)
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Summary/Overview

Under this award the fluid mechanics measurement capabilities of the combustion and fuels laboratory of the University of Southern California were upgraded notably. Thus, the needs for determining flame properties of fundamental and practical importance can be met readily. The experimental data so obtained will be used for the validation of chemical kinetic and diffusion models for hydrocarbon fuels used in air-breathing devices that are of interest to the Air Force; furthermore, the data contain important information related to the performance of various practical fuels and will be useful in defining the operational range of advanced propulsion systems, such as scramjets. The acquired instrumentation involves high-resolution, high-accuracy laser-based systems and subsystems and constitutes a major improvement of current capabilities in the principal investigator’s (PI’s) laboratory. This improvement enhances the quality of ongoing research that is conducted under AFOSR support significantly. Three state-of-the-art velocity measurement systems were developed to complement an existing digital particle image velocimetry (DPIV) system that was acquired previously under AFOSR support. The first velocity measurement system is a compact laser Doppler velocimeter (LDV). The other two are DPIV systems, which were developed around a high-power YAG laser that is available to the PI at no cost to AFOSR. After determining the velocity fields in flames, fundamental flame properties can be derived, such as laminar flame speeds, as well as ignition and extinction limits. The sensitivity of those properties to both chemical kinetics and molecular transport can be large, so that validation and/or optimization of various models can be achieved. The parameter space of the PI’s ongoing research is extensive, as it involves a large number of fuels, such as neat hydrocarbons, jet fuels and their surrogates, fuel-air ratios, initial reactant temperatures, and thermodynamic pressures.

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14. ABSTRACT
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Technical Discussion
1.0 Introduction
1.1 General Aspects of Laminar Flame Experiments

Current trends in combustion science and technology focus largely on the reliable modeling of high-speed reacting flows in complex geometries. In addition to the hardware limitations of current computer technology to handle the large number of dependent variables in simulations of realistic reacting configurations, large uncertainties exist in the oxidation kinetics of hydrocarbons even at the C_2 level (*e.g.*, Egolfopoulos & Dimotakis 2001), and those uncertainties are more profound for the heavier C_7-C_{16} hydrocarbons. Studies in homogeneous systems provide useful information for the oxidation/pyrolysis kinetics of fuels. Past experience in combustion science has shown that in many instances, kinetic schemes developed in homogeneous systems fail to predict fundamental flame properties by large factors (*e.g.*, Egolfopoulos & Dimotakis 2001). Recent studies (Dong et al. 2005; Holley et al. 2006; 2007) have revealed that validating chemical kinetic models can be complicated further by uncertainties associated with the diffusion coefficients. More specifically, it has been shown that under conditions of relevance to ignition, burning, and extinction of flames of heavy hydrocarbons, the sensitivities of global flame properties to the diffusion coefficient can be of the same order or higher than the sensitivities to the rate constants. This issue has not been addressed in detail and deserves more emphasis. Current kinetics models have been developed without considering the attendant effects of diffusion. In order for a kinetic mechanism to be reliable, its validation must be comprehensive, which requires the prediction of experimental observations in homogeneous systems and flames. In flames, a kinetic mechanism is tested in environments of large temperature and species concentration gradients, which constitutes a more "integrated" test compared to homogeneous reactors.

The validation of mechanisms in flames is associated with a number of challenges such as:

1. Accurate description of the experimental boundary conditions
2. Establishing laboratory flames that are:
    a. One dimensional;
    b. Laminar;
    c. Steady;
    d. Planar or smooth;
    e. Adiabatic or non-adiabatic with well characterized heat losses;
    f. Affected by fluid mechanics in a well controlled manner;
3. Obtaining measurements that are accurate with satisfactory spatial and temporal resolutions.

The Stagnation Flow Configuration

Among all experimental configurations, stagnation flows have been shown to be the most meritorious ones as they can satisfy the conditions stated above closely (*e.g.*, Law 1988; Kee et al. 1988). In the last 20 years substantial advances have been made in combustion science and technology through systematic flame studies conducted in stagnation flows. The most profound example is the development of the GRI mechanism (Smith et al. 2000) describing the CH_4 oxidation kinetics, which eventually became the "industry standard" for natural gas combustion. Flame data obtained in stagnation flows were used extensively in the development of the various versions of the GRI mechanism.

In addition to implementing the stagnation flow configuration, the quality of the reported data depends notably on conceptual and experimentation considerations. Conceptually, the fundamentals of combustion science must be implemented in order to derive important flame properties such as, for example, laminar flame speeds and/or ignition/extinction limits.

Stagnation flow data can be used to derive the "true" laminar flame speed. The extrapolation technique proposed by Law (*e.g.*, Wu & Law 1984; Law 1988) has been used extensively to derive laminar flame speeds, and subsequent improvements of the technique were made (*e.g.*, Vagelopoulos et al. 1994; Chao et al. 1997) that further improved the accuracy of the results. Subsequently, Vagelopoulos & Egolfopoulos (1998) advanced an alternative method to determine laminar flame speeds "directly" by allowing a flame to undergo a transition from a positively stretched planar, stagnation state to a negatively stretched, Bunsen state.

The stagnation flow configuration can be used also to provide fundamental data on flame ignition and extinction limits. The ignition studies of Law and coworkers (*e.g.*, Fotache et al. 1995; 1997; 2000) were conducted by counterflowing fuel/inert jets against a heated airjet. Alternatively, Egolfopoulos and coworkers (e.g., Langille et al. 2006) determined fundamental ignition limits by counterflowing fuel/inert jets against vitiated air that was produced by the combustion of ultra-lean H_2/air mixtures. In both approaches, the ignition limits were determined as the maximum temperature at the hot boundary for a given strain rate and fuel concentration in the fuel jet. Law and coworkers (*e.g.*, Law et al. 1986; Law 1988), as well as Egolfopoulos and coworkers (*e.g.*, Egolfopoulos 1994; Holley at al. 2006; 2007), have utilized the stagnation flow configuration to determine extinction limits experimentally that are of fundamental value. More specifically, extinction strain rates have been determined for a variety of reacting mixtures and initial thermodynamic conditions.

The experimental laminar flame speeds, as well as the ignition and extinction limits that are obtained in stagnation flows, can be modeled directly, and their sensitivity to rate constants, as well as to molecular diffusion, is notable (*e.g.*, Dong et al. 2005; Fotache et al. 1995; 1997; 2000; Holley at al. 2006; 2007). Thus, these global experimental data constitute an important database against which models can be validated and/or optimized.

Laser Doppler Velocimetry and Digital Particle Image Velocimetry in Flames

Experimentally, laminar flame speeds, ignition limits, and extinction limits can be obtained with non-intrusive measurements of the flow field using laser Doppler velocimetry (LDV) and/or digital particle image velocimetry (DPIV). Both techniques have relative advantages and disadvantages. An increased level of accuracy often characterizes LDV measurements, especially if the signal-to-noise ratio of the bursts of scattered light is high, and if a large number of bursts are averaged. Both of these requirements can be met readily with the current technology in receiving optics and signal processors. The accuracy of LDV has been confirmed in the PI's laboratory through independent tests against velocity data obtained in non-reacting flows through the use of hot-wire anemometry. Implementing a DPIV system in flames and achieving the level of accuracy of LDV is a challenge, particularly when accuracy of the order of 1-2% is required. This stringent accuracy is dictated by the fact that uncertainties of the order of 5% or higher in laminar flame speed for example, are not desirable, as important information pertaining to chemical kinetics can be masked by such large uncertainty bars. Implementing DPIV for determining flow velocities in flames within the 1-2% range requires a non-trivial optimization of light power, image sensor properties, seeding particle size and concentration, receiving optics, and processing algorithms, as well as the post-processing procedures.

If optimized carefully and performed properly, DPIV in flames can achieve similar, or even better, accuracy than LDV measurements. Extensive comparisons between LDV and DPIV measurements have been made in the PI's laboratory using an in-house DPIV system that was developed under AFOSR support and a recently-acquired (under NASA support) mini-LDV system that is used for NASA-related flame research. During these comparisons, it is always best for a laboratory to be equipped with both LDV and DPIV, as occasional comparisons between results obtained for the same conditions using both approaches can provide a greater degree of confidence in the reported results. Furthermore, two-dimensional effects can be captured with DPIV more readily, while measurements through the dilatation zone can be achieved better with LDV, which outperforms DPIV for low particle number densities, such as in regions of low gas-phase density.

1.2 Combustion Research with Neat Fuels, Jet Fuels, and their Surrogates

The combustion research that the PI is performing under AFOSR support aims to provide insight into the physical and chemical processes that control the burning behavior of neat and practical complex fuels that are relevant to air-breathing propulsion. AFOSR supports this research as follows:

1. **Grant**: FA9550-07-1-0168
   - **Title**: *Experiments and Reaction Models of Fundamental Combustion Properties*
   - **Duration**: 4/1/07 – 11/30/09
   - **PI**: Fokion N. Egolfopoulos (University of Southern California)
   - **Co-PI**: Hai Wang (University of Southern California)
   - **Amoun**t: $660,000 (total for the 3-year period)

2. **Grant**: FA9550-08-1-0040
   - **Title**: *Development of Detailed and Reduced Kinetics Mechanisms for Surrogates of Petroleum-Derived and Synthetic Jet Fuels*
   - **Duration**: 3/1/08 – 11/30/10
   - **PI**: Fokion N. Egolfopoulos (University of Southern California)
   - **Co-PIs**:
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     - Craig T. Bowman, Ronald K. Hanson, Heinz Pitsch (Stanford University)
     - Chung K. Law (Princeton University)
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     - R. Peter Lindstedt (Imperial College London) at no cost
     - Wing Tsang (National Institute of Standards and Technology) at no cost
   - **Amount**: $2,100,000 (total for the 3-year period)

This research involves combined experimental and detailed numerical studies of a number of fundamental combustion phenomena and properties. Experimentally, the phenomena of flame ignition, propagation, and extinction, as well as flame structures of systematically chosen fuel/oxidizer mixtures, are being considered and characterized. The studies include both small (gaseous) and large (liquid) hydrocarbon molecules in view of their importance towards the accurate description of the combustion behavior of practical fuels. These studies expand notably the parameter space of existing archival fundamental combustion data. Theoretically, the detailed modeling of the experimental data, along with available literature experimental data, is performed by using well-established numerical codes and reaction and transport models that are developed based on a novel approach. More specifically, deriving reliable kinetics models is based on the following four specific objectives: (a) to develop and test a suitable array of mathematical and computational tools that can be used to quantify the joint rate parameter uncertainty space and, in doing so, to facilitate the rational design of reaction models suitable for any given target fuel or a mixture of these fuels; (b) to examine the applicability of the $H_2/CO/C_{1-4}$ reaction model, developed under the current support, to predict the phenomena of flame ignition, propagation, and extinction along with flame structures; (c) to examine the effect of inelastic collisions on binary diffusion coefficients; and (d) to test the hypothesis that there exists a critical reaction model for use as the quantitative kinetic foundation for modeling higher hydrocarbon combustion. The main goal of this research is not only to produce a comprehensive reaction model suitable for air-breathing propulsion simulations but also to generate a set of new approaches and computational tools for rational reaction model development and optimization.

The parameters considered in the experiments include the fuel type, reactant composition, flame temperature, and combustion mode. Hydrogen, carbon monoxide, single-component gaseous and liquid hydrocarbons, as well as jet fuels and their surrogates, are studied experimentally in the counterflow configuration. The measurements include largely laminar flame speeds, as well as ignition and extinction limits. Important results have been produced and published already for fuels ranging from H_2 to jet fuels and their surrogates (*e.g.*, Dong et al. 2002; 2005; Holley et al. 2006; 2007).

While experiments with gaseous fuels can be performed with relative ease, using liquid fuels, especially heavy ones, requires special care. More specifically, given their low vapor pressure, the reactants must be heated to temperatures that are typically close to their boiling point so that they can be maintained in the vapor phase for the duration of the experiment. Basic kinetic arguments and recent experimental evidence obtained in the PI’s laboratory (e.g., Holley et al., 2007) suggest that improper fuel heating and mixing (with the inert and/or oxidizer) method can result in modification of the fuel composition through either thermal cracking or partial oxidation. Thus, the combined effect of fuel temperature and residence time at any given temperature needs to be considered carefully in the experiments in order for the derived data to be reliable and archival. The issues related to heavy liquid fuels have been resolved in the PI’s laboratory based on experience gained during the last 6 years of ongoing research.

The parameter space that must be investigated for all fuels and conditions is very large, as shown in Table 1. The three flow velocimeters that were acquired under the present support, will allow for the prompt completion of the proposed experiments.

A. Fuels (*total 34*):

Neat (23): H_2, CO, CH_4, C_{2x} (3), C_{3x} (3), C_{4x} (3), *n*-$C_{5\text{-}14}$ (10), *iso*-C_8
Jet (7): JP7, JP8, JP10, RP1, JetA, Coal-Derived, Fisher-Tropsch
Surrogates (4): Two-, three-, six-, twelve-component mixtures

B. Combustion modes (*total 2*): Premixed, non-premixed

C. Phenomena considered (*total 3*): Ignition, extinction, propagation (premixed only)

D. Equivalence ratios for premixed flames (*total 10*): 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, 1.5

E. Fuel mass fraction in fuel-inert stream for non-premixed flames (*total 6*): 0.05, 0.1, 0.25, 0.5, 0.75, 1.0.

F. Thermodynamic pressures (*total 4*): 1.0, 2.0, 4.0, 8.0 atm

Table 1: *Approximate parameter space involved in the PI's AFOSR-supported research on neat fuels, jet fuels, and their surrogates. The subscripts indicate carbon numbers, and the numbers inside the parentheses indicate the number of cases considered.*

Any realistic combination of the numbers shown in Table 1 can result in an excessively large amount of experimental data. Certain measurements, such as those required to determine laminar flame speeds, may require the determination of at least 20 velocity fields to yield one laminar flame speed value. At least 100 to 200 velocity fields need to be determined per investigator per day in order to derive laminar flame speeds for all cases considered within a reasonable time. The determination of ignition and extinction limits can be determined in a more direct manner based on a new "direct" approach that the PI and his group have advanced recently (Holley et al. 2006). While fewer velocity profiles need to be determined in the ignition and extinction studies, additional time is required to identify the critical conditions of ignition and extinction so that fluid mechanics measurements are performed subsequently.

Finally, the parameter space shown in Table 1 represents what is required ideally to provide data for mechanism validation/optimization. The PI and his group, however, have established combined experimental and theoretical approaches that guide the experiments so that certain regimes of the overall parameter space are eliminated if they do not offer any new information for model validation/optimization. Thus, the approach that is taken in the PI's laboratory is not to scan every single parameter range and potentially waste resources but instead to assess parameter ranges that could provide worthwhile insight into the controlling physical and chemical processes that are relevant to air-breathing propulsion. This approach has resulted in several successes, including a recent one in which it has been shown that propagation and extinction of heavy hydrocarbons and jet fuels are controlled largely by C_1-C_4 kinetics, while the $C_{>5}$ kinetics practically play no major role (Ji et al. 2009; You et al., 2009). In summary, the parameter space can be reduced intelligently, but still the number of experiments that need to be conducted remains very large.

2.0 Summary of Equipment

2.2 Mini Laser Doppler Velocimetry (mini-LDV)

A one-dimensional mini-LDV integrated with a computer-controlled traversing system was acquired. A nearly identical system has been acquired recently under NASA support, and it has been shown to perform very well in the counterflow configuration. The mini-LDV system is a product of Measurement Science Enterprise, and its compact size and relative low price makes it a very attractive option for flame experiments under both atmospheric and elevated pressures.

The main features of the mini-LDV are:

- Integrated diode laser of 120 mW continuous power. Unlike other commercial LDV instruments, the laser is hard-mounted and integrated inside the probe, requiring no user alignment and adjustment. The diode laser has an average lifetime of 10,000 operational hours.
- The optical design's unique (patented) features are:
    - No on-site calibration by the user is needed as the entire optical probe is sealed permanently.
    - No laser wavelength stabilization is required, as the optical design automatically compensates for any changes in the wavelength of the diode laser resulting from changes in the laser temperature.
    - The mini-LDV has a high optical efficiency, resulting in a high laser power density at the probe volume.
    - The mini-LDV has a smallest possible probe volume dimension, resulting in high spatial resolutions.
    - The mini-LDV is designed mechanically to withstand high vibration and thermal loadings.
- The signal processing consists of the following components:
    - 100 MHz, National Instrument Digital PC board
    - Hardware and software based on fast signal digitization and FFT-based processing. Zero padding, interpolative peak detection and high resolution FFT are used to calculate the Doppler frequency from the analog output of the photo detector.

2.2 Digital Particle Image Velocimetry (DPIV)

Three new DPIV systems were developed to complement an existing DPIV system developed previously under AFOSR support. These new systems enhance greatly the current capabilities of the PI's laboratory largely through improvements in imaging sensor technology and processing algorithms. Two of these new systems were developed around a single double-pulsing YAG laser that has become available to the PI at no cost to AFOSR. The existing system was enhanced also through software and optics upgrades, so that it can function as two independent systems, resulting in four DPIV systems. The two new systems that were developed use similar software but differ significantly in the imaging hardware. The asymmetry in the imaging systems provides an enhanced range of measurement capabilities. Specifically, the two cameras were chosen for their relative merits in light sensitivity and resolution, and the optical systems for both illumination and imaging differ accordingly. One system has a high-resolution, low frame rate camera, while the second has a lower resolution ultra-sensitive high framing rate camera. Both cameras are Pelitier cooled, and the imaging objectives are specific to high magnification and light sensitivity, respectively. Some of the key aspects of the new systems and their integration with the existing equipment are discussed below.

Improved flexibility in laboratory

The DPIV experiments are carried out at greater than 1:1 magnification, requiring precise optical alignment of both the illumination and imaging optics. Complete alignment of the optical system can take substantial effort to reproduce, and any movement or alterations to the configuration between different ensembles of a given experimental data set could introduce small discontinuities that would render the entire ensemble unusable. Hence it is highly desirable that, for maximum throughput, each burner configuration has a dedicated measurement system.

Cost efficiency

Updating of the existing system while adding two higher performance systems was achieved in a cost efficient way through sharing of a BigSky double pulsing PIV-01 YAG laser ($40,000), which was acquired recently at no cost to AFOSR or DoD, and the construction of a simple flipping-mirror/beam-splitter assembly that allows the two independent DPIV systems to share the same laser. This experimental arrangement was possible as two of the new burner rigs were installed at either end of the same optical table, where their relative alignment remains constant. Laser power could be provided to each system independently or to both systems simultaneously (at half power). This configuration also allows for the two DPIV systems to share a single USB timing box, economizing an additional $8,700.

Increased magnification

Improvements to the laser light sheet and camera lens systems, as well as the increased camera resolution, allows higher magnifications (1:3), providing spatial resolution better than 10 microns per velocity vector or 2 microns for planar laser-induced fluorescence (PLIF) of CH.

Reduced turn-around-time through higher speed processing and optimization

Even for fully configured and optically aligned DPIV systems, the time from image acquisition to data output (turn around time) can be quite long. Limitations in image quality, algorithm choice, algorithm efficiency, ease of use, and CPU power all will be addressed with the newly developed systems.

Improved accuracy

The accuracy of the velocity measurements improved notably through the adoption of the new software from LaVision Inc., which has performed excellently in the recent PIV Challenge (http://www.pivchallenge.org/). The ability to use in-house custom algorithms with the acquired commercial software package was an important aspect in its selection. Such algorithms have been developed at USC over the past 15 years and allow the DPIV technique to be adapted to very specific measurement challenges, such as moving flame fronts and complex turbulent flow phenomena. Other recent enhancements include the ability to vary the processing parameters locally as a function of both the local seeding particle concentration and the local strain rate.

Enhanced light sensitivity

The acquired newer generation cameras have increased greatly the light sensitivity. Specifically, the PCO Sensicam QE, which has 65% quantum efficiency and is thermo-electrically cooled down to -12°C, allows extremely low image noise on the order of 4 e-rms. These cameras are well suited for measurement techniques other than DPIV, such as planar laser-induced fluorescence (PLIF) of CH that can measure the location of the flame front accurately, while obtaining the velocity field with DPIV.

Multi-scale hierarchical approach

Hierarchical adaptive grid algorithms that can be optimized to measure strain rates along specific directions and even provide for nested measurements were implemented in the newly developed systems (Fincham & Delerce 2000). These techniques have shown extreme robustness to low particle seeding densities and strong velocity gradients, making them well suited for the PI's longer-term research objectives.

3.0 Description of Acquired Equipment

Two types of equipment were purchased. The relative merits and complementary functionality have been described above. The components of the first system, the mini-LDV, are detailed below.

	Item	Units	Company	$/Unit	Total Price
Mini-LDV	**1D MiniLDV-FG-100 Probe**	1	Measurement Science Enterprise	$19,250	$19,250
	BP-LDV Burst Processor System	1	Measurement Science Enterprise	$14,762	$14,762
	Desktop PC Computer	1	Measurement Science Enterprise	$1,640	$1,640
	1-D Translation Stage with Support Structure	1	Measurement Science Enterprise	$6,292	$6,292
	Traversing Supporting Stand	1	Measurement Science Enterprise	Included	Included
	Educational Discount		Measurement Science Enterprise		-$1,700
	Sales Tax (8.25%)				$3,320
	Sub-Total				**$43,564**

This mini-LDV system has been integrated successfully into the PI's laboratory and is functioning as anticipated.

The second type of equipment was digital particle imaging velocimetry (DPIV), aided by the acquisition of a Quantel Laser from sources external to this proposal and some creative sharing of both software and hardware. Three systems were added to an existing one. All four systems also were standardized.

Details of the actual components purchased are outlined below.

	Item	Units	Company	$/Unit	Total Price
DPIV	**Imager *Intense* cross-correlation CCD camera**	2	LaVision Inc.	$17,745	$35,490
	Programmable Timing Unit (PTU-9); External	2	LaVision Inc.	$9,135	$18,270
	DaVis Software package (USB port dongle) - Version 7.2,	2	LaVision Inc.	$4,725	$9,450
	2D PIV/PTV Software package	2	LaVision Inc.	$13,125	$26,250
	PIV System Installation	1	LaVision Inc.	$2,000	$2,000
	Shipping, Handling, and Documentation	1	LaVision Inc.	$300	$300
	Educational Discount		LaVision Inc.		-$29,528.00
	Sales Tax (8.25%)				$5,299.14
	PC Computer for acquisition software	2		$775	$1,750
	PCO Pixelfly Camera	2	The Cooke Corporation	$8,619	17,238.20
	Sub-Total				**$ 86,519.34**

Total expenditure for mini-LDV and DPIV systems $130,083

4.0 Equipment Use

The **1D MiniLDV-FG-100 Probe** system was mounted to the **1-D Translation Stage with Support Structure** and structural aluminum framing to traverse the flames in the vertical direction**. The BP-LDV Burst Processor System** was integrated directly to the probe through installation on the host PC computer. The system was calibrated and shown to deliver accurate results for moderate traverse speeds. Measurement Science and Technology performed on-site installation and training for the PI's laboratory staff and students.

The DPIV system cameras were mounted on **SherLine 2D** traverses fitted with **Manfrotto Tripod heads,** allowing 5 degrees of freedom in a robust and stable mount. The two Peltier cooled **PCO** cameras were shared with the existing **NewWave** Laser through a smart beam-sharing arrangement and the non-cooled Gig-E **PixelFly PCO** cameras were set up to share the **Quantel** laser. Each pair of cameras and their corresponding laser were wired into a single USB **LaVision PTU** timing box to share a single **LaVision** acquisition license through partitioning of the dongle with a USB switch. The arrangement allowed seamless switching between the different experiments. **The LaVision** representative gave a one-day tutorial session to all potential operators. Overall data acquisition and processing times have been reduced by an order of magnitude, and the data quality has been shown to be comparable, if not better, than the prior "home-built system."

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